Device and Process Modeling in Microelectronics and Nanoelectronics

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Vision

- To develop a highly integrated and intelligent simulation environment that facilitates the rapid development and validation of next-generation electronic devices as well as associated materials and fabrication processes through virtual prototyping at multiple levels of fidelity

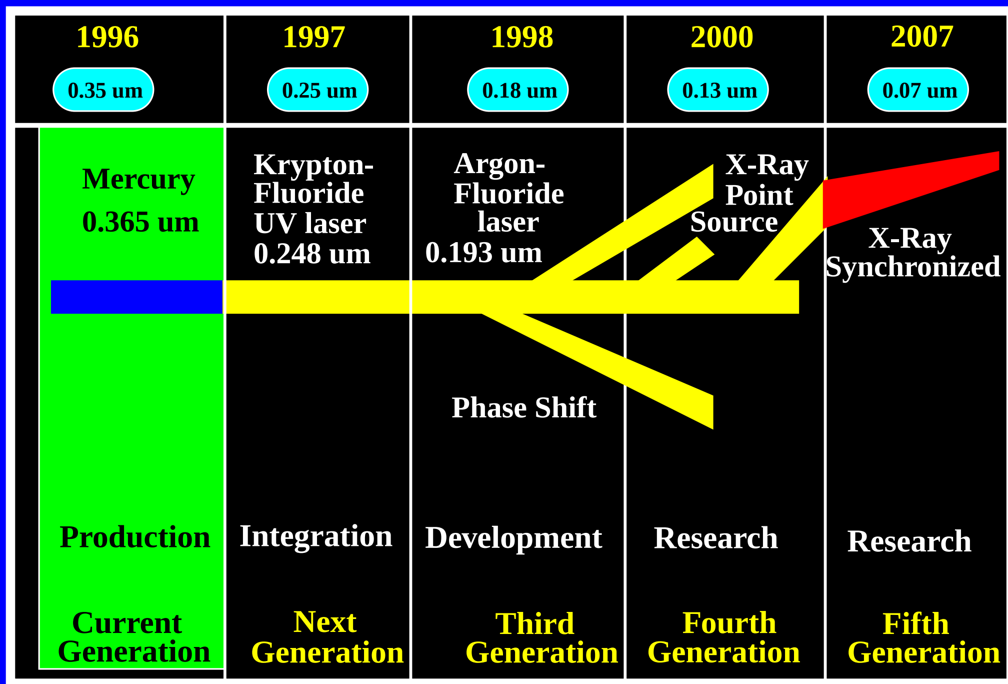
Research Objectives

- Develop physical models to simulate new devices useful for NASA missions
- Develop computational framework based on advanced parallel algorithms and embed them into number of new emerging technologies
- Develop and deploy an intelligent simulation environment through the transparent and seamless integration of underlying Information Technology components

Devices and Applications

- Devices
  - Submicron and deep-submicron devices (ULSI)
  - Quantum devices
  - Optoelectronic devices
  - Micro-Electro-Mechanical (MEM) and ASIM devices ASIM
- Applications
  - Future high-performance computer systems
  - Smart spacecraft
  - Smart aircraft control systems
  - Air traffic management systems
  - High speed data communications
  - Optical storage
  - Optical sensors

Roadmap for Semiconductor Industry



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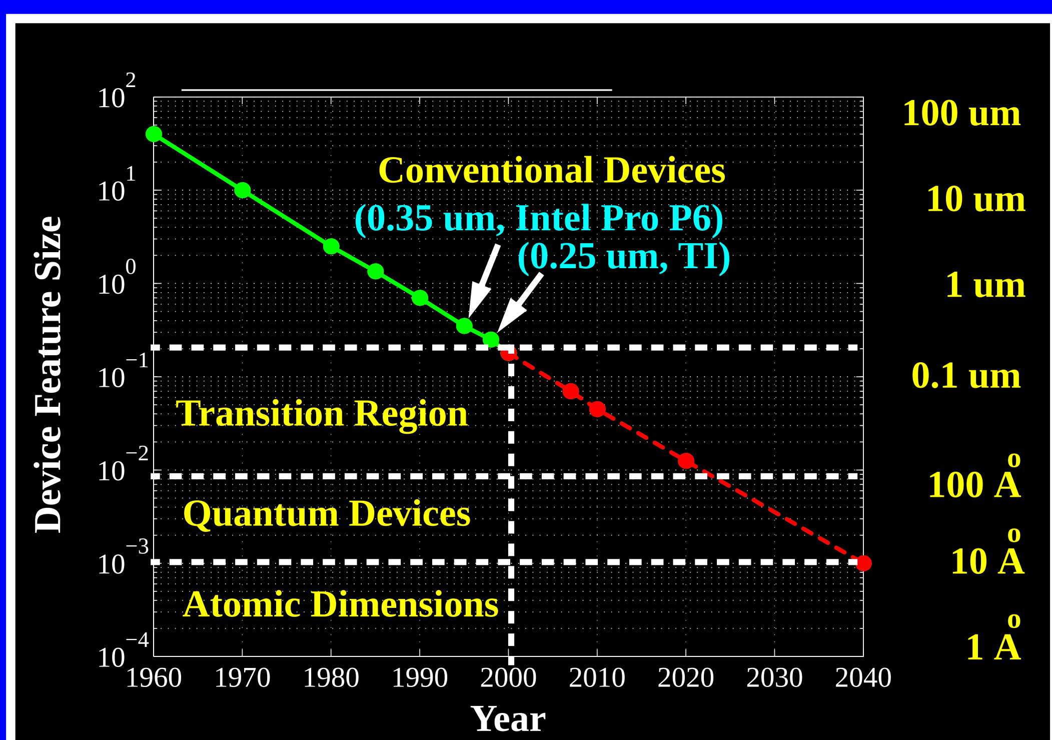
Quantum Devices



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NASA HPC Requirements

- **High-Performance Computers**

  Ultrafast computers for critical missions

- **Low-powered**

  Higher Tflops/Pflops per watt

- **Ultra Compact**

  Higher Tflops/Pflops per square foot

- **Resistant to Radiation Damage**

  The NASA Remote Exploration and Experimentation Project: High Performance Computing in Space

Benefits of Technology Modeling

- Design times may be reduced in half
- Advanced technologies can be investigated "on-the-fly"
- Physical prototypes can be eliminated
- Initial design quality can be improved, resulting in significant life-cycle cost reductions
- Basic understanding of the device operation through 3-D visualization
- Vastly less expensive than experiment
- Modify device and test conditions at will

Higher-Level Technical Approach

- Physical models framework
  - Semiclassical methods
  - Quantum mechanical methods
- Computational framework
  - PDE/Integrals based methods
  - Particle based methods
- Information Technology framework
  - Hardware
  - Software

Physical Models Framework

Microscopic Methods

Stochastic Methods
Fullband Monte Carlo
Reduced Band MC

Deterministic Methods
Scattering matrix
Cellular Automata

Non-equilibrium Methods
Green's Functions

Macroscopic Methods

Series Expansion Methods
Spherical Harmonics
Laugurre Polynomials

Moment Methods
Classical HD
Quantum HD

Energy Transport Methods
Drift-diffusion
Energy Balance

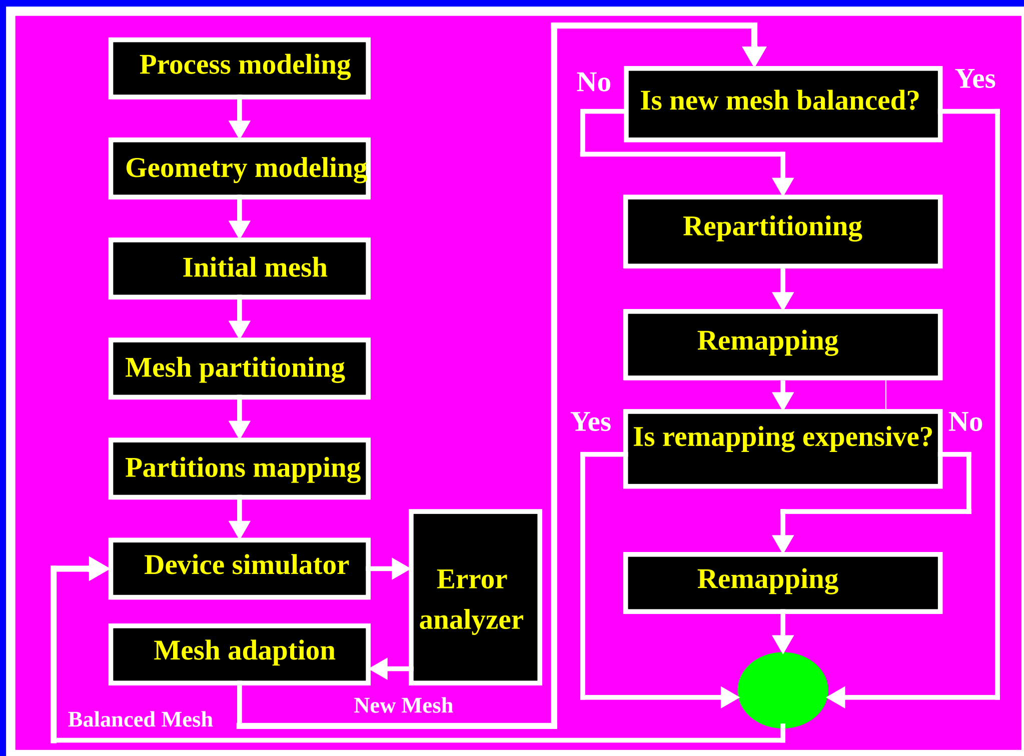
Computational Framework

- PDE/Integral equations based methods
  - Multilevel algorithms
  - Fully adaptive methods
  - Unstructured mesh methods
  - Level set methods
- Particle methods
  - Gridless methods
  - Gridded methods
- Scalable Algorithms
  - Latency tolerant algorithms
  - Data locality
  - Load balance methods

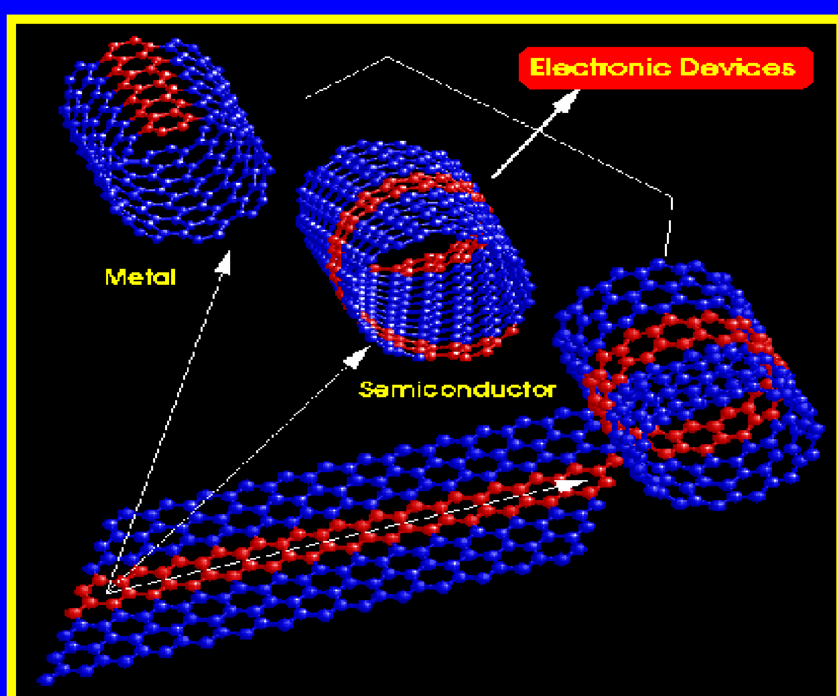
Information Technology Framework

- Hardware
  - Parallel computers
  - Mass storage devices
  - Virtual reality systems
  - High speed networks
- Software
  - Computational steering capability
  - Databases/Data management systems
  - Distributed computing environments
  - Artificial intelligence/Expert systems
  - Visualization software
  - Graphical user interfaces

Parallel Adaptive Device Simulator

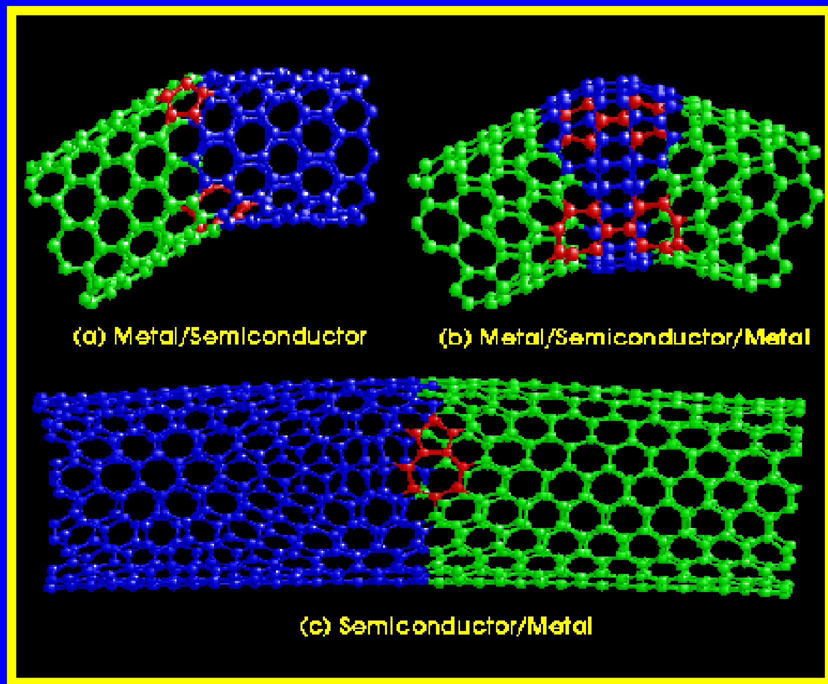


Metallic and Semiconductor Single-Walled Carbon Nanotubes



Jie Han, 1997

Fullerene-based Hetero-junctions

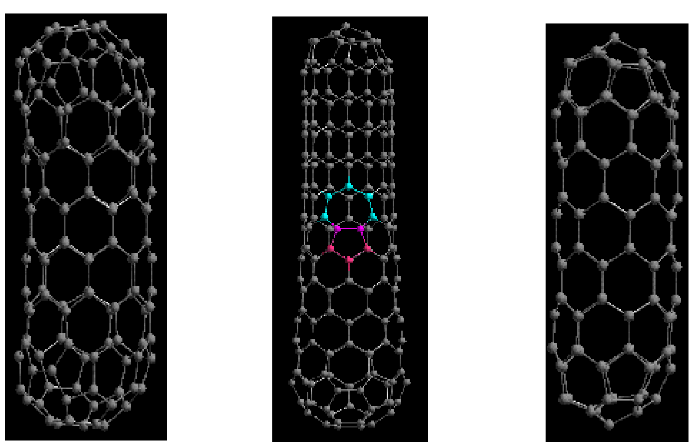


Jie Han, 1997

Nanotube Hetero-junction

Example: Carbon Nanotube Switch

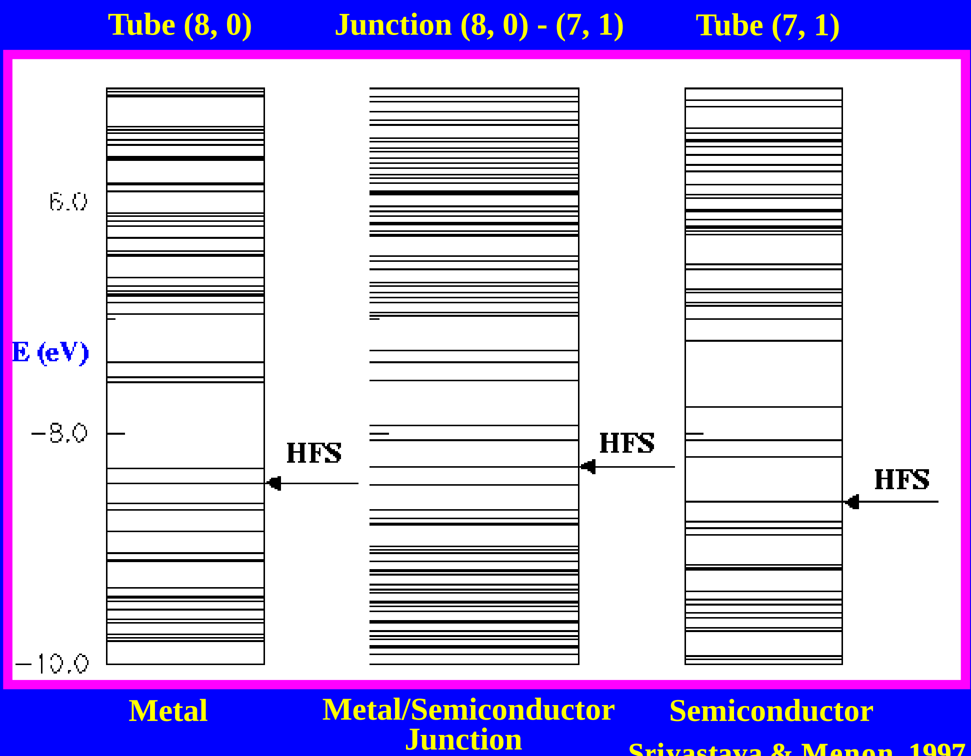
Tube (8,0) Junction (8,0)-(7,1) Tube (7,1)



Metalic Metal/Semiconductor Junction Semiconducting

Srivastava & Menon, 1997

Bandstructure of Nanotubes



Srivastava & Menon, 1997